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Adaptive Computation and Modeling for Multiscale Analysis

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13. ABSTRACT (Maximum 200 words)

Algorithms and software for the adaptive solution of multiscale problems involving partial differential equations and linkage to atomic level simulations. Efforts focused on techniques for using the discontinuous Galerkin method to solve hyperbolic and singularly perturbed parabolic problems. New anisotropic adaptive and parallel solution techniques, *a posteriori* error estimation strategies, limiting procedures that reduce spurious oscillations near discontinuities, and discontinuity detection strategies that reduce the need for limiting, thereby reducing both excess diffusion and spurious oscillations were developed. The software and methods are being tested on a variety of problems involving compressible flows. In collaboration with engineers at Benét Laboratories, we have been investigating muzzle blast from cannons with perforated brakes.

A new procedure to couple atomic/continuum level adaptive simulations was developed and demonstrated on test problems. Scale error indicators have developed and adaptive construction of local atomic regions demonstrated.

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Statement of Problem Studied

Algorithms and software for the adaptive solution of multiscale problems involving partial differential equations and linkage to atomic level simulations were researched. Techniques for using the discontinuous Galerkin method to solve hyperbolic and singularly perturbed parabolic problems were developed. New anisotropic adaptive and parallel solution techniques, *a posteriori* error estimation strategies, limiting procedures that reduce spurious oscillations near discontinuities, and discontinuity detection strategies that reduce the need for limiting, thereby reducing both excess diffusion and spurious oscillations were developed. The software and methods are being tested on a variety of problems involving compressible flows. In collaboration with engineers at Benét Laboratories, we have been investigating muzzle blast from cannons with perforated brakes.

A new procedure to couple atomic/continuum level adaptive simulations was developed and demonstrated on test problems. Scale error indicators have developed and adaptive construction of local atomic regions demonstrated.

Summary of Most Important Results

Discontinuous Galerkin Methods

An adaptive software system for solving multiscale hyperbolic conservation laws by the discontinuous Galerkin (DG) method has been developed. The software is capable of addressing problems in one, two, and three spatial dimensions using anisotropic adaptive h-refinement.

The DG method offers several advantages relative to traditional finite element and finite volume methods when solving hyperbolic systems of conservation laws. The advantages and several aspects of the DG method are described in a sequence of manuscripts that construct orthogonal bases [18,21], describe limiting procedures [10], develop efficient local time stepping algorithms [5,18], create efficient serial and parallel data representations [20], and apply the method to compressible flow problems [2,3,18,22].

In order to guide adaptive enrichment and appraise the accuracy of computed solutions, we developed *a posteriori* estimates of discretization errors. We show [1, 9] that the leading term of the spatial discretization error of a piecewise-polynomial solution of degree p is the difference between orthogonal polynomials of degrees p and $p + 1$. In one dimension, the orthogonal polynomials are Radau polynomials and in two dimensions on triangular elements they are linear combinations of Dubiner polynomials. We further demonstrate a strong superconvergence at downwind element boundaries where the average spatial error converges as $O(h^{2p+1})$ [9].

The strong superconvergence at outflow boundaries can be used to identify discontinuities. This, in turn, can be used to provide information on where to apply limiting to reduce oscillations when using high-order methods. This procedure has been remarkably successful at reducing both excess dissipation and spurious oscillations near discontinuities [10].

To increase the effectiveness of the adaptive procedures a set of anisotropic adaptive mesh control technologies have been developed. The two key components of this procedure are anisotropic correction indication procedures and anisotropic mesh adaptation procedures. The anisotropic correction procedure has two major components [22] that construct a anisotropic mesh metric tensor over the problem domain. In smooth portions the mesh metric tensor employs the Hessian of the solution field [12,13,22]. The portions of the domain that are not smooth employ the shock capturing procedure of reference [10]. In these locations the mesh metric tensor is defined to align with the shocks and to blend into the smooth portions of the domain [22]. The anisotropic mesh adaptation is carried out using a complete set of mesh modification operations for anisotropic meshes [12,13] and fully account for curved domain boundaries [11].

Figures 1 and 2 show a 2-D and 3-D result obtained with the adaptive anisotropic adaptive DG procedure just described.

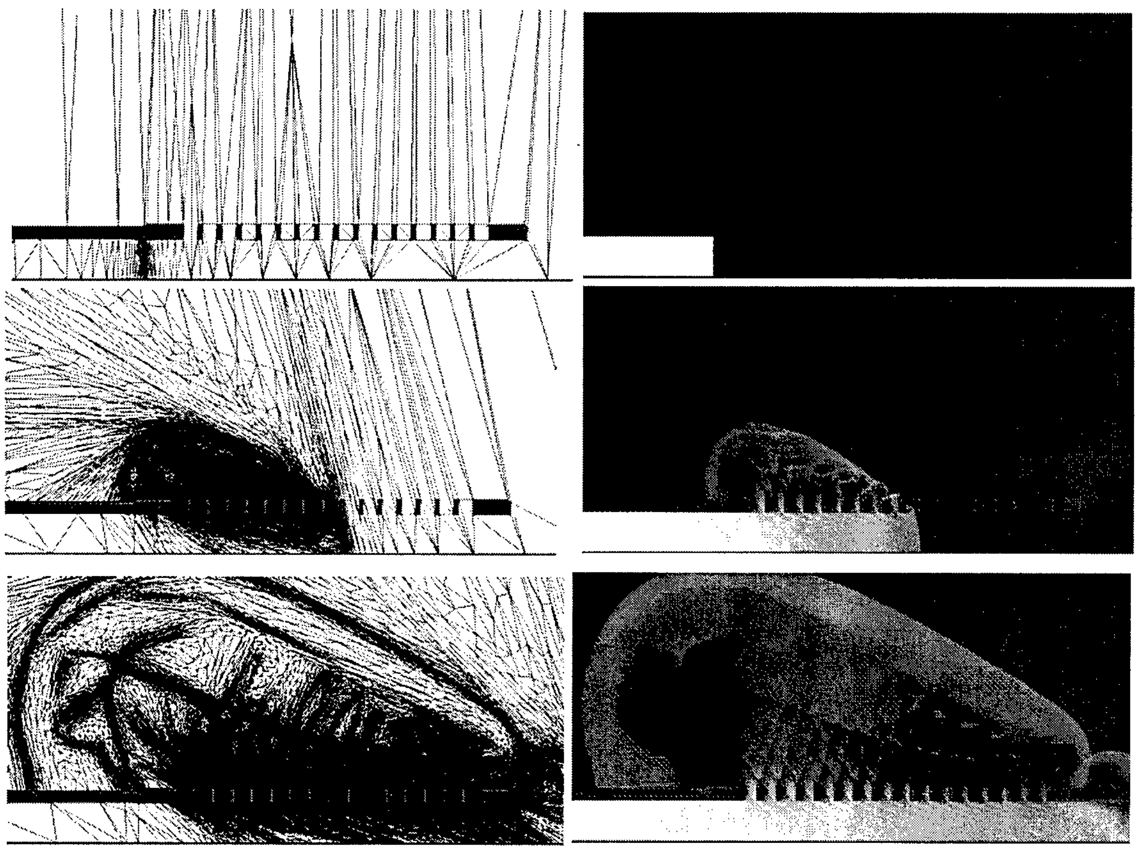


Figure 1. The meshes and pressure contours for t=0.0, t=0.0002 and t=0.0005 in a 2-D Muzzle blast simulation.

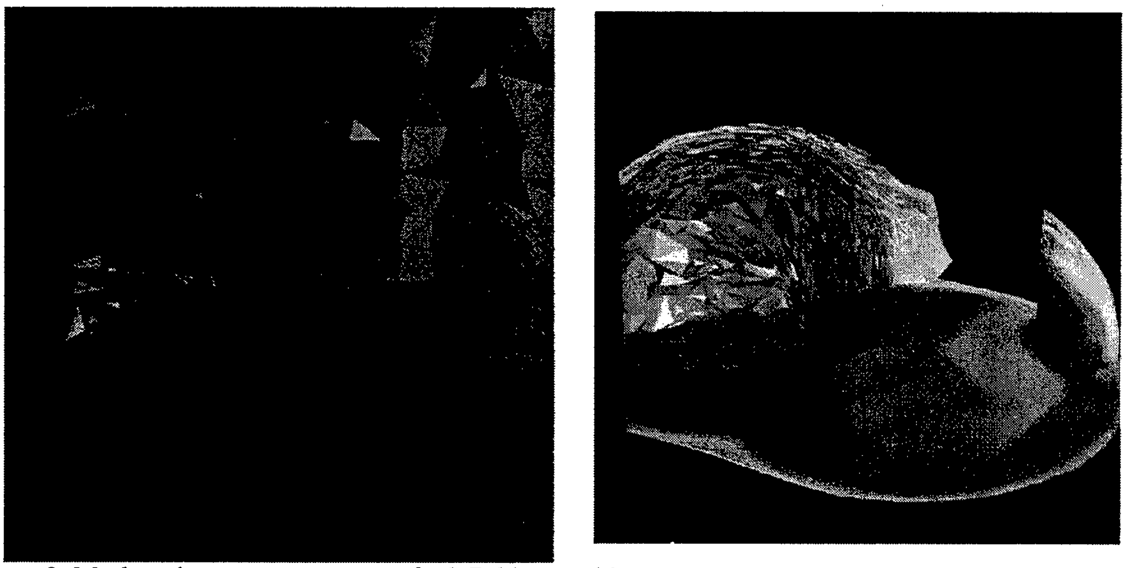


Figure 2. Mesh and pressure contours of a 3-D blast problem.

Level Set Method for Solving Fluid/Rigid body Interaction Problems

The simulation of flow problems with moving objects require an effective means to account for the motion of the object through the domain of the mesh. A level set based method that allows the object to move through the mesh has been developed to allow rigid objects to move through a mesh. In this method an Eulerian mesh is created over the entire computational domain [6]. The movement of the rigid object will cut some of the mesh entities and introduce new boundaries inside the fluid. The level set technique is used to track the interface between the rigid body and the compressible fluid, and the Ghost Fluid Method (GFM) to capture the correct boundary condition implicitly at the interface. Therefore, handling the boundaries is simplified and we have the advantage of doing a fluid calculation on the entire domain. By doing this, we can handle the contribution of the embedded moving boundaries in the fluid without mesh modification.

For the elements in the Eulerian mesh, there are two different possible cases according to their position with respect to the zero level set of the level set function. Case (i), the entity is totally outside the zero level set. Case (ii), the entity is totally inside the zero level set or the entity is cut by the zero level set. For all entities of case (i), the object in the fluid has no direct effect on this entity, so no special operations are needed. For all entities of case (ii), the boundary of the fluid/solid interface must be accounted for using the GFM to capture the correct boundary conditions. The level set enables us to locate those entities that need special treatment, even when we do not know the position of the precise position of the moving boundary in the entity. Actually, we also do not want to find the precise position of the moving boundary because it is an expensive operation, especially for high order approximation and for high dimension case.

We treat the rigid body moving in a fluid as a contact discontinuity at the interface because the fluid near the interface will move with the velocity of the rigid body. The Rankine-Hugoniot

jump conditions imply that both the pressure and the normal velocity are continuous across the interface. Therefore, we set the values for the *ghost entity* to enforce these two conditions. There are three kinds of state variables that need to be set: velocity, density, energy (or pressure). At the same time, since the interface of the rigid body acts as a reflective wall boundary for the fluid, a reflective constraint can capture the boundary condition. For DGM, ghost values are set at every *ghost entity* by considering and setting the values at every gauss point inside the rigid object.

This approximation is straightforward even in the multi-dimensional case. This is an advantage because we can treat the one-, two-and three-dimensional cases with the same scheme and the numerical implementation is simple and consistent for all cases. On the other hand, a lot of reflective points may need to be searched. To speed the procedure, an octree data structure is designed and implemented. In the case that a reflective point does not belong to the computational domain of the problem, specific care must be taken in setting values.

This procedure has been combined with adaptive mesh refinement [21,22] to control solution errors to solve problems with moving objects (see Figure 3).

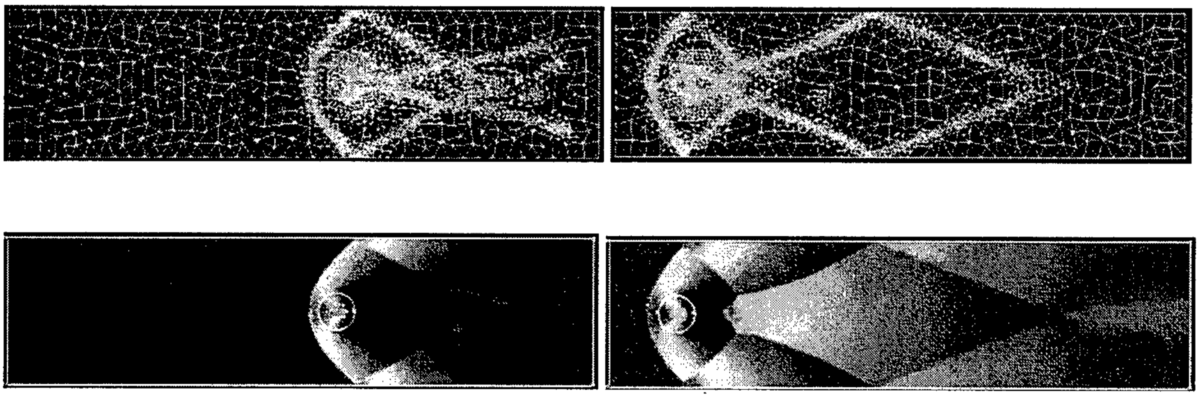


Figure 3. Example sphere moving through a fluid domain.

Coupled Atomistic-Continuum Simulations

We have developed a Composite Atomistic-Continuum Method (CACM) for multiscale analysis of coupled discrete and continuum models [5]. The main idea of the method is to use atomistic analysis only at places where needed to capture the highly nonlinear behavior and continuum analysis will be used elsewhere for efficiency. Such a method permits the explicit representation of the nano-scale physics. The components of the CACM and its development include:

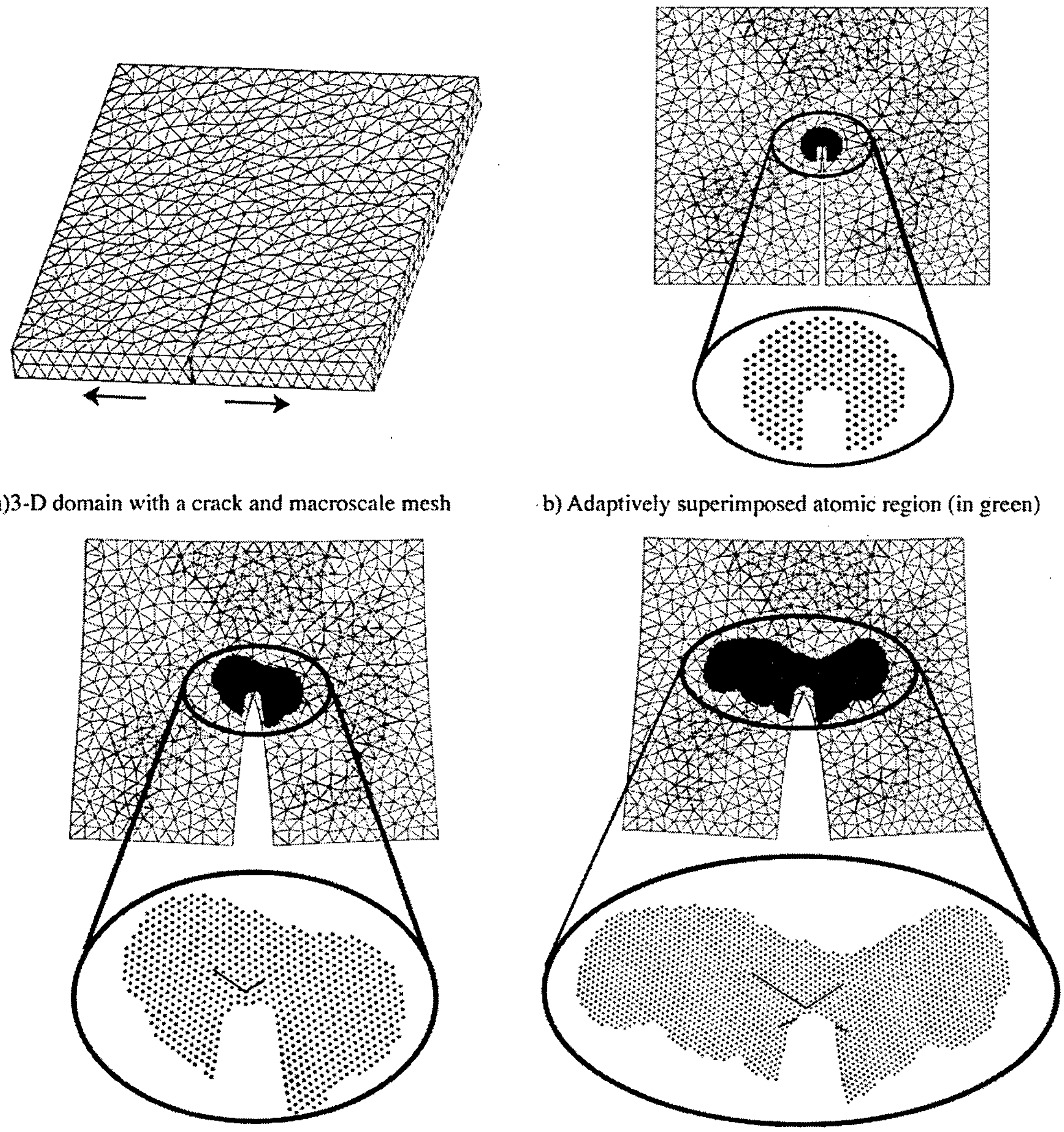
1. *CACM Method:* In CACM, the continuum is represented by linear elasticity model, and discretized using finite elements on a coarse grid. An atomistic representation in the regions of high field gradients or where the highly nonlinear and non-local behavior of the lattice is important, *i.e.*, at the places where there is nucleation or close range interaction of the defects is used. In these regions, an atomistic grid is used which carries the boundary conditions imposed by the continuum and returns to the continuum correcting information. The atomistic grid is defined in restricted spatial regions and

relocates with the defects. This procedure minimizes the computational effort associated with atomistic simulations, while insuring the required accuracy at relevant spatial locations. We have tried various algorithms, and operators to link the two scales. Based on the effectiveness, meaningfulness and ease of transferring the information from the continuum to the atomistic, and back to the continuum, at this point we have selected to transfer the displacement information from the continuum to the atomistic as the boundary condition for the atomistic analysis. Then in turn the atomistic analysis provides the correction of the continuum solution at the critical places. The atomistic grid is overlaid on the continuum grid, and this method doesn't have the restriction of matching the two grids. This allows for using quite coarse grid at the continuum level unlike some other methods, which is forced to use refined meshes for the continuum near the atomistic regions to match the atomistic grid.

2. *Implementation of the CACM:* The algorithm for the CACM was implemented in the environment of Trellis, a framework for 3D adaptive multi-physics and multi-scale analysis. The Trellis framework was extended to build the scope for multiscale applications. The capability to solve 3D atomistic problems using various types of potentials was implemented within the Trellis framework. To couple the continuum analysis with the atomistic analysis a module responsible for transferring the information between the two analyses was implemented. This module has been implemented in a general manner so as to be able to be utilized for possible coupling of other analyses.
3. *Error indicators:* We have identified the following three criterions required for the adaptive selection of the model:
   (a) Non linearity: This is characterized by the magnitude of the strain. We have already developed an error indicator to capture this property. The error indicator is based on the relative magnitude of the first order energy term in comparison to the zeroth order term.
   (b) Non locality: This is characterized by the gradient of the strain. Indicators to capture this information were proposed, and used effectively in their method.
   (c) Non-convexity: This is characterized by the change in energy felt by the continuum once a defect passes through it.
4. *Adaptive modeling:* The software has to be generalized in the following respects to handle adaptivity: (a) Building a module that will provide indicators of the error in modeling. (b) Automatic generation of the discrete regions based on the error information.
5. *Demonstration of the CACM:* Figure 4 shows an example of the multiscale modeling of the growth of defects at a crack tip [5].

Technology Transfer

Joseph E. Flaherty and Mark S. Shephard have regular interactions with Robert Dillon, Deborah Bleau, and Daniel Cler of Benét Laboratories [2,3]. As described in Section 1, we have been collaborating on using the DG software to analyze muzzle blast effects with large-calibre weapons systems. These problems involve complex three-dimensional interior and exterior flows including realistic geometries and ground reflections.



a)3-D domain with a crack and macroscale mesh b) Adaptively superimposed atomic region (in green)

Figure 4. Example of the multiscale modeling of the growth of defects at a crack tip.

J. E. Flaherty was also the dissertation advisor (with Henry Nagamatsu) of Eric Kathe, a mechanical engineer at Benét Laboratories. Dr. Kathe completed his Ph.D. dissertation in May 2002.

A start-up company, Simmetrix Corporation, is building on the mesh modification and analysis framework developments done in this project. Simmetrix has commercialized a number of the mesh generation and mesh adaptation procedures developed in this project. They have also obtained two ARMY supported SBIR's. The first is concerned with the development of commercial parallel adaptive simulation technologies. The second, which has just recently started is concerned with the development of multiscale simulation technologies with an

emphasis on atomic level simulation model generation and control. Rensselaer is a sub-contractor to Simmetrix on both of these SBIR's.

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Scientific Personnel

In addition to the Principal Investigators Joseph E. Flaherty and Mark S. Shephard, former Ph.D. scholar Lilia Krivodonova and Ph.D. students Peng Hu, Jamal Faik, Viswanath Ramakkagari and Jianguo Xin have also received support. Dr. Krivodonova completed her Ph.D. dissertation in August 2002 and is currently a Postdoctoral Fellow at New York University's Courant Institute of Mathematical Sciences. Dr. Xin completed his thesis in April of 2005, and Peng Hu, Jamal Faik and Viswanath Ramakkagari are writing their thesis'.

Inventions

No patents were filed based on this work.